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On the corrections of the measured integrated Bragg reflections due to thermal diffuse scattering

By NANNY NILSSON

With 3 figures in the text

SUMMARY

The contribution of the diffuse scattering to the measured intensity of a Bragg reflection has been computed for some reflections of sylvin and rock-salt, assuming width of slits and angles of rotation corresponding to the experiments made by James and Brindley [1] and Renninger [2].

It is evident that the contribution of the diffuse scattering to the measured integrated reflections amounts to considerable values (up to 30 % for the highest reflections), and thus cannot be neglected as has been thought until now.

The measured integrated reflection can, as to the dependence of the Bragg angle v_0, be written as the real integrated Bragg reflection times a factor $\exp\left(\text{const}\,\frac{\sin^2 v_0}{\lambda^2}\right)$, due to the effect of the diffuse scattering. This fact explains why good agreement can be obtained between theoretically calculated F values and those obtained from intensity measurements and experimentally determined Debye–Waller factors.

Introduction

The effect of the thermal motion on the scattering of X-rays by crystals has been investigated by Debye [3], Faxén [4] and Waller [5]. In his dissertation Waller gives the complete formula for the scattering by small crystals. In a later work [6], he has derived an expression for the integrated intensity of the diffuse maxima, coinciding with the Bragg maxima. The present calculations are to be considered as an extension of Waller's paper.

For a simple cubic crystal, containing a large number of unit cells, but yet so small that the absorption within it may be neglected, the following formulas for the intensity are valid:

$$\left.\begin{aligned} J &= J_1 + J_2, \\ J_1 &= \frac{I}{R^2}\,|F|^2\,e^{-2M}\,T_0, \\ J_2 &= \frac{I}{R^2}\,|F|^2\,e^{-2M}\sum_{\nu=1}^{\infty} T_\nu. \end{aligned}\right\} \quad (1)$$

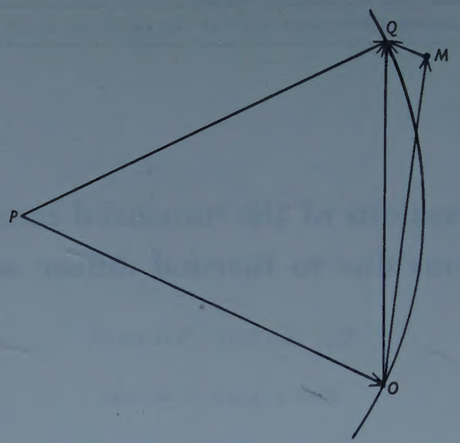

Fig. 1.

I is the intensity of the incident monochromatic, plane wave, J the scattered intensity. J_1 is the Bragg intensity modified by the temperature factor e^{-2M}. J_2 represents the diffuse temperature scattering. R is the distance from the crystal to the point, where the intensity is observed. F is the atomic scattering factor. T_0 is the Laue interference function. T_1 represents scattering where only one elastic wave is involved. It has pronounced maxima at the reciprocal lattice points. The scattering corresponding to $\sum_{\nu=2}^{\infty} T_\nu$ forms a nearly uniform background with only slight maxima and may thus be neglected for our purposes.

In Fig. 1 the sphere of reflection is drawn for a direction of incidence PO. The lattice wave that gives the contribution represented by T_1 to the scattering in the direction PQ has the wave vector $2\pi \overrightarrow{MQ} = 2\pi \mathrm{g}$, M being the reciprocal lattice point lying nearest to Q (Faxén–Waller vector condition).

Our task is to calculate the energy, corresponding to J_2, received by a slit, placed in the direction of Bragg reflection, when the crystal is rotated through the Bragg position with uniform angular velocity, around an axis, lying in the reflecting crystal plane and perpendicular to the wave normal of the incident wave. From the formulas (72), (65) and (62″) in Waller's dissertation we get the following expression for T_1, valid for small values of ϱ:

$$T_1 = \frac{\varkappa^2 k T N}{a \varrho^2} \frac{A}{B}, \tag{2}$$

where

$$A = (\alpha - \alpha_0)^2 [b_1 (c_{11} + c_{12}) \bar\beta^2 \bar\gamma^2 + c_{44} (c_{11} - c_{44}) (\bar\beta^2 + \bar\gamma^2) + c_{44}^2] + \text{cycl. perm.} -$$
$$- 2 (\alpha - \alpha_0)(\beta - \beta_0)(c_{12} + c_{44}) \bar\alpha \bar\beta (b_1 \bar\gamma^2 + c_{44}) + \text{cycl. perm.}$$

$$B = b_1^2 b_2 \bar\alpha^2 \bar\beta^2 \bar\gamma^2 + b_1 (c_{11} + c_{12}) c_{44} (\bar\alpha^2 \bar\beta^2 + \bar\beta^2 \bar\gamma^2 + \bar\gamma^2 \bar\alpha^2) + c_{11} c_{44}^2$$

λ = the wave length of the incident X-rays

$\varkappa = 2\pi/\lambda$

k = Boltzmann's constant

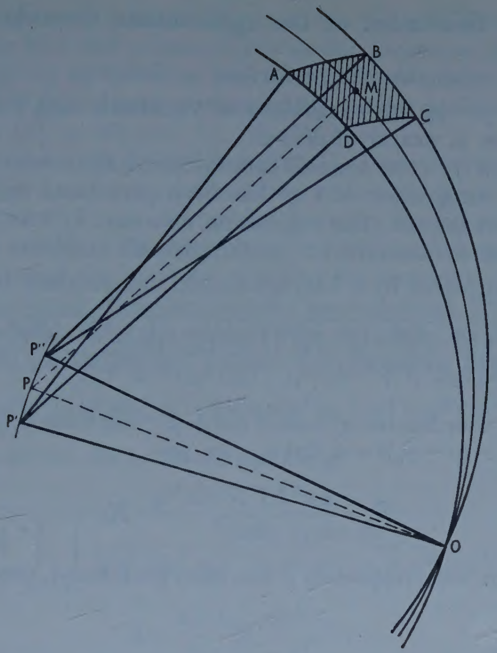

Fig. 2.

T = temperature

N = number of atoms in the crystal

a = distance between adjacent atoms in the lattice

$\varrho = 2\pi a/\bar{\lambda} = 2\pi a\,|\mathrm{g}|$, where $\bar{\lambda}$ is the wave length of the elastic wave

$\bar{\alpha}$, $\bar{\beta}$, $\bar{\gamma}$ are the direction cosines of g referred to the crystallographic axes.

α_0, β_0, γ_0, and α, β, γ are the direction cosines of respectively the incident and the scattered X-rays referred to the same axes.

$b_1 = c_{11} - c_{12} - 2c_{44}$, $b_2 = c_{11} + 2c_{12} + c_{44}$.

c_{11}, c_{12}, and c_{44} are the elastic constants.

Fig. 2 shows a section of the region in the reciprocal lattice space, through which the integration of T_1 has to be performed. The direction of the incident X-rays is changed from $P'O$ to $P''O$ during the rotation of the crystal. Thus the sphere of reflection moves from AD to BC nearly parallel to itself in the neighbourhood of the reciprocal lattice point M. The angles $AP'D$ and $BP''C$ correspond to the angular width of the slit. The height of the slit corresponds to an extension of the region of integration perpendicular to the plane of the section in Fig. 2. Thus the endpoint of the vector g moves in an approximately parallelepipedal space, when the crystal is rotated. To perform the exact integration of T_1 would be a very lengthy numerical work. The actual calculations are made according to the following approximate method.

Derivation of the approximate formula

The approximate evaluation is performed as follows:

1. $\alpha-\alpha_0$, $\beta-\beta_0$, $\gamma-\gamma_0$ are considered as constant, and the same as when the Bragg condition is exactly fulfilled.
2. A mean value of T_1 over a small sphere round M is calculated.
3. The remaining integration of $1/\varrho^2$ has been performed by Waller [6], assuming infinite height of the slit. The expression obtained by him is used here, and the error introduced on account of the infinite slit height is estimated.

Denoting the mean value by a bar, we obtain immediately from (2)

$$\overline{T}_1=\frac{\varkappa^2 kTN\,\overline{[(\alpha-\alpha_0)^2+(\beta-\beta_0)^2+(\gamma-\gamma_0)^2]\,\{b_1(c_{11}+c_{12})(\bar{\alpha}^2\bar{\beta}^2+\bar{\beta}^2\bar{\gamma}^2+\bar{\gamma}^2\bar{\alpha}^2)+c_{44}(2c_{11}+c_{44})\}}}{3a\varrho^2\,[b_1^2 b_2\,\bar{\alpha}^2\bar{\beta}^2\bar{\gamma}^2+b_1(c_{11}+c_{12})\,c_{44}\,(\bar{\alpha}^2\bar{\beta}^2+\bar{\beta}^2\bar{\gamma}^2+\bar{\gamma}^2\bar{\alpha}^2)+c_{11}c_{44}^2]}\,.$$

Introducing polar coordinates $\bar{\alpha}=\sin\theta\cos\phi$, $\bar{\beta}=\sin\theta\sin\phi$, $\bar{\gamma}=\cos\theta$ and putting $(\alpha-\alpha_0)^2+(\beta-\beta_0)^2+(\gamma-\gamma_0)^2=4\sin^2 v_0$, we get

$$\overline{T}_1=\frac{4\varkappa^2 kTN\sin^2 v_0}{3a\varrho^2}\cdot\mathcal{K}.$$

When the integration with respect to ϕ has been performed, the following expression for $\mathcal{K}$ is obtained

$$\left.\begin{aligned}\mathcal{K}=&\frac{A}{\sqrt{CD}}\operatorname{arctg}\sqrt{\frac{C}{D}}+\\&+2\int_0^1\frac{(BD-AE+BCx^2+ACx^4-ACx^6)\,dx}{(Cx^2+D)\sqrt{\begin{aligned}&4E^2+ED+(6ED+D^2+EC)x^2+(D^2+CD-7ED-2EC)x^4+\\&+(EC-5D^2-3CD)x^6+(3CD+3D^2)x^8-CDx^{10}\end{aligned}}}\,.\end{aligned}\right\}$$

$x=\cos\theta$,

$A=b_1(c_{11}+c_{12})$, $\quad C={b_1}^2 b_2$, $\quad E=c_{11}c_{44}^2$,

$B=c_{44}(2c_{11}+c_{44})$, $\quad D=b_1(c_{11}+c_{12})c_{44}$.

A simple formula derived by taking the mean values of each of the terms in the numerator and the denominator of (3) separately gives a good approximation of $\mathcal{K}$.

$$\mathcal{K}_{\text{appr}}=\frac{\frac{1}{5}b_1(c_{11}+c_{12})+c_{44}(2c_{11}+c_{44})}{\frac{1}{105}b_1^2 b_2+\frac{1}{5}b_1(c_{11}+c_{12})c_{44}+c_{11}c_{44}^2}\,.$$

Table 1

$T°$ abs	KCl			NaCl		
	$\mathcal{K}\times 10^{11}$	$\mathcal{K}_{\text{appr}}\times 10^{11}$	Error %	$\mathcal{K}\times 10^{11}$	$\mathcal{K}_{\text{appr}}\times 10^{11}$	Error %
86	2.228	2.112	−5.2	1.418	1.403	−1.1
280	2.464	2.368	−3.9			
290	2.480	2.385	−3.8	1.594	1.588	−0.4

Table 1 shows a comparison between $\mathcal{K}_{\text{appr}}$ and the value of $\mathcal{K}$ obtained by numerical evaluation of (5). For KCl the values of the elastic constants given by Durand [7] and for NaCl those given by Overton and Swim [8] are used.

The integration of $1/\varrho^2$ has been performed by Waller as follows. (For details see Waller's dissertation [5], p. 53, and l.c. [6].)

On account of the vector condition for g (Fig. 1) ϱ^2 may be expressed as a function of the angles u, w, and φ. u and w are defined from the equations $u = V_0 - v_0$, $v = V - v_0$, $w = u + v$, where V_0 and V are the angles between respectively the incident and the scattered X-rays and the reflecting plane. φ is the angle between two planes, one containing the direction of the incident rays and the normal to the reflecting plane, and the other the scattering direction and the same normal. Thus u corresponds to the rotation of the crystal, w to the width of the slit and φ to the height of the slit. The expression for ϱ^2, valid for small values of u, w, and φ is given by

$$\varrho^2 = \varkappa^2 a^2 (4u^2 \sin^2 v_0 - 4uw \sin^2 v_0 + w^2 + \varphi^2 \cos^2 v_0).$$

The surface element of the slit is $R^2 \cos v_0 \, dw \, d\varphi$.

Introducing

$$\sigma = \frac{1}{\pi} \int_{u_1}^{u_2} \int_{w_1}^{w_2} \int_{\varphi_1}^{\varphi_2} \frac{\cos v_0 \, du \, dw \, d\varphi}{4u^2 \sin^2 v_0 - 4uw \sin^2 v_0 + w^2 + \varphi^2 \cos^2 v_0}$$

and putting
$$K = \frac{4\pi k}{3a} \mathcal{K} \frac{\sin^2 v_0}{\lambda^2} T,$$

we get the following expression for the integrated diffuse intensity

$$\frac{E_2 \omega}{I} = \frac{|F|^2 e^{-2M}}{\Delta^2} K \lambda^2 a \sigma \delta V \tag{6}$$

written in conformity with Darwin's formula for the integrated Bragg reflection

$$\frac{E_1 \omega}{I} = \frac{|F|^2 e^{-2M}}{\Delta^2} \frac{\lambda^3}{\sin 2v_0} \delta V. \tag{7}$$

ω is the angular velocity of the crystal during the rotation, Δ is the cell volume $= a^3$, and $\delta V = Na^3$ is the volume of the crystal piece. E_1 and E_2 are the total energies corresponding respectively to J_1 and J_2 entering through the slit during the rotation. Assuming the slit very long and thus putting

$$\varphi_1 = -\infty, \qquad \varphi_2 = +\infty,$$

σ is given by

$$\left.\begin{aligned} \sigma = \frac{w_2}{2\sin^2 v_0} \left[f\left(\frac{2u_2 \sin^2 v_0}{w_2}\right) - f\left(\frac{2u_1 \sin^2 v_0}{w_2}\right) \right] - \\ - \frac{w_1}{2\sin^2 v_0} \left[g\left(\frac{2u_2 \sin^2 v_0}{w_1}\right) - g\left(\frac{2u_1 \sin^2 v_0}{w_1}\right) \right] - (u_2 - u_1) \ln \left(-\frac{w_1}{w_2}\right). \end{aligned}\right\} \tag{8}$$

Here

$$\begin{aligned} f(x) = x \ln \left[(1-x) \sin v_0 + \sqrt{x^2 - 2x \sin^2 v_0 + \sin^2 v_0}\right] - x + \\ + \sin v_0 \ln \left[x - \sin^2 v_0 + \sqrt{x^2 - 2x \sin^2 v_0 + \sin^2 v_0}\right]. \end{aligned}$$

$g(x)$ is obtained from $f(x)$ if $\sin v_0$ is replaced by $-\sin v_0$. If w_1 and w_2 are both positive, one has to replace g with f in the second brackets, and to put $+w_1/w_2$ instead of $-w_1/w_2$ in the last term.

Denoting the total energy entering through the slit during the rotation by E, we get

$$E = E_1 + E_2 \quad \text{and} \quad \frac{E\,\omega}{I} = \frac{E_1\,\omega}{I}(1+\alpha)$$

where

$$\alpha = \frac{a}{\lambda} \sin 2\,v_0\,K\,\sigma. \tag{9}$$

Comparison with experiments

The experimental values, used for comparison, are results from measurements with mosaic crystals. The formula for the integrated Bragg reflection is in that case obtained by replacing δV with $(2\,\mu)^{-1}$ in (7), μ being the ordinary linear absorption coefficient of the crystal, and I being the total energy incident per unit time on the crystal. In the comparison below we use the expression (9) for α, which means that we assume the same orientation for all the elements in the crystal mosaic.

Measurements made by James and Brindley [1]

Table 2 gives the value of α for the reflections of KCl used by James and Brindley to determine β in the expansion

$$M = \frac{8\,\pi^2 \sin^2 v_0}{\lambda^2}\left(\beta\,T + \frac{\gamma}{T} + \frac{\delta}{T^3}\right) \tag{10}$$

deduced by Waller [5]. In this expression γ does not depend on the atomic forces, and can be calculated directly. δ depends on the atomic forces, but can be estimated with sufficient accuracy, since the term containing it is very small. The values are

$$\gamma = 1.075 \times 10^{-17}, \qquad \delta = -0.56 \times 10^{-14}.$$

In reality β is determined from the following formula:

$$\frac{\Delta M}{h^2+k^2+l^2} = \frac{2\,\pi^2}{a^2}\left\{\beta\,(T_1 - T_2) + \gamma\left(\frac{1}{T_1} - \frac{1}{T_2}\right) + \delta\left(\frac{1}{T_1^3} - \frac{1}{T_2^3}\right)\right\} \tag{11}$$

(h, k, l are the Miller indices of the crystal plane), where

$$\left(\frac{E\,\omega}{I}\right)_{T_2=86^\circ} \Big/ \left(\frac{E\,\omega}{I}\right)_{T_1=290^\circ} = e^{2\,\Delta M}.$$

The measurements are made with Mo K_α radiation ($\lambda = 0.71$ A) and the angles involved are $u_2 = -u_1 = 1^\circ\!.25$, $w_2 = -w_1 = 0^\circ\!.75$.

To account for the general background scattering James and Brindley rotated the ionization chamber 2° from the Bragg position and made measurements altering the angles of rotation correspondingly. The values thus obtained were subtracted from the main results. In our calculations we have to make the corresponding correction, which we call σ'. The angles are $u_1 = 0^\circ\!.25$, $u_2 = 2^\circ\!.25$, $w_1 = 1^\circ\!.25$, $w_2 = 2^\circ\!.75$. An estimation of the errors introduced in σ and σ' assuming infinite slit height gives the result that they cancel each other approximately. Thus

$$\sigma_{\text{corr}} = \sigma - \sigma'.$$

The last column of Table 2 shows a very interesting feature of the effect studied. For each temperature we can write

$$M = \text{const}\ \frac{\sin^2 v_0}{\lambda^2}.$$

The diffuse scattering has the effect of reducing the constant by a certain amount, when M is determined from measurements of the integrated Bragg reflection. Table 3 shows the values of ΔM obtained by James and Brindley and the same values corrected with respect to the influence of the diffuse scattering.

Table 2

Spectr.	$\frac{\sin^2 v_0}{\lambda^2}\ A^{-2}$	σ	σ'	$\sigma_{\text{corr}} = \sigma - \sigma'$	α $T = 290^\circ$	α $T = 86^\circ$	$\frac{\ln(1+\alpha)}{\sin^2 v_0/\lambda^2}\ A^2$	
							$T = 290^\circ$	$T = 86^\circ$
400	0.1016	0.178	0.036	0.142	0.037	0.010	0.358	0.098
600	0.2285	0.148	0.035	0.113	0.097	0.026	0.405	0.112
444	0.3047	0.138	0.038	0.100	0.129	0.034	0.398	0.110
800	0.4062	0.129	0.036	0.093	0.179	0.048	0.406	0.115
10.00	0.6347	0.117	0.036	0.081	0.282	0.075	0.391	0.114
666	0.6855	0.115	0.037	0.078	0.298	0.079	0.380	0.111
						M.V.	0.390	0.110

Table 3

Spectr.	$h^2+k^2+l^2$	ΔM	Correction	ΔM_{corr}	$\frac{\Delta M_{\text{corr}}}{h^2+k^2+l^2}$
400	16	0.107	0.013	0.120	0.00750
600	36	0.242	0.034	0.276	0.00767
444	48	0.344	0.044	0.388	0.00808
800	64	0.450	0.059	0.509	0.00795
10.00	100	0.714	0.088	0.802	0.00802
666	108	0.786	0.093	0.879	0.00814
					M.V. 0.00789

James and Brindley obtain

$$\beta = 7.25 \times 10^{-21} \quad \text{corresponding to } M = 1.688\ \frac{\sin^2 v_0}{\lambda^2}\ A^{-2}.$$

After correction of their ΔM values our result is

$$\beta = 8.11 \times 10^{-21} \quad \text{corresponding to } M = 1.885\ \frac{\sin^2 v_0}{\lambda^2}\ A^{-2}.$$

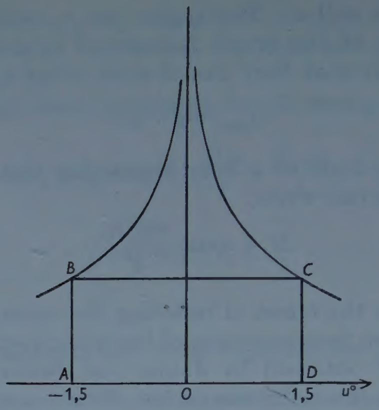

Fig. 3.

The measurements are, however, not very good. Indeed if we use the theoretical values of the atomic scattering factors F_{K^+} and F_{Cl^-} and compute $M\left(\frac{\sin^2 v_0}{\lambda^2}\right)^{-1}$ for each temperature, we do not get the desirable constancy. The constancy of $\Delta M/(h^2+k^2+l^2)$ is, however, satisfactory, so the value of ΔM and thus the experimental value of M should be better than each of the single measurements.[1]

Renninger's measurements [2]

Renninger has made measurements on rock salt at room temperature and the temperature of liquid hydrogen. However, the value of the low temperature seems to be very uncertain, so we have only considered the measurements at room temperature. Renninger has registered the reflection curves and made the integration of them. Using the theoretical values of the atomic scattering factors F_{Na^+} and F_{Cl^-} he calculated the separate temperature factors M_{Na^+} and M_{Cl^-} and also determined the best common M-value for sodium and chlorine. He also made the reverse calculation using the values of F_{Na^+} and F_{Cl^-}. Plotting these values against $\sin v_0/\lambda$ he obtained curves which agree very well with the theoretical F-curves. Indeed, at room temperature they coincide. However, in calculating the characteristic temperature Θ, corresponding to his common M-value, from the well-known formula

$$M=\frac{6h^2T}{mk\Theta^2}\left\{\Phi(x)+\frac{x}{4}\right\}\frac{\sin^2 v_0}{\lambda^2} \tag{12}$$

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[1] We found that $M\left(\frac{\sin^2 v_0}{\lambda^2}\right)^{-1}$ at room temperature was decreasing from 2.56 (400) to 1.75 (666). It was thus constantly higher than the value 1.69 obtained by James and Brindley from $\Delta M/(h^2+k^2+l^2)$. At 86° K the value goes from 1.40 down to 0.61 for the same reflections. The discrepancy of the single measurements from the expected values can be explained by the presence of an absorbing surface layer on the crystal, the possibility of which was pointed out by James and Brindley. The lowest reflections must give the largest absorption and in calculating ΔM for each reflection the error is eliminated.

—where $\Phi(x)$ is the Debye function of $x = \Theta / T$ and m is the mean value of the atomic masses for chlorine and sodium—he obtained the very high value of $\Theta = 319°\,\mathrm{K}$.

As appears in Renninger's paper he has used a very wide slit, about 5°, and made the integration between the limits $\pm 1°.5$. Fig. 3 shows our approximation of the actual reflexion curve for the diffuse scattering.

We should subtract from our σ-values a correction σ' corresponding to the rectangular area $ABCD$ in Fig. 3. As will be pointed out later the single points of the curve are more uncertain than is the integral of the curve. Thus the value of σ' is more uncertain than the value of σ. Even in this case the corrections due to the infinite slit height cancel each other when we take the difference $\sigma - \sigma'$. The results are given in Table 4.

Table 4

$h\,k\,l$	$\frac{\sin^2 v_0}{\lambda^2} A^{-2}$	σ	σ'	$\sigma_{\mathrm{corr}} = \sigma - \sigma'$	α	$\frac{\ln(1+\alpha)}{\sin^2 v_0/\lambda^2} A^2$
222	0.0947	0.321	0.217	0.104	0.015	0.157
400	0.1263	0.306	0.202	0.104	0.024	0.188
600	0.2841	0.269	0.166	0.103	0.077	0.261
622	0.3473	0.261	0.157	0.104	0.103	0.282
444	0.3789	0.257	0.153	0.104	0.117	0.292
800	0.5051	0.246	0.143	0.103	0.171	0.313
644	0.5367	0.244	0.142	0.102	0.183	0.313
822	0.5683	0.242	0.140	0.102	0.197	0.316
10.00	0.7983	0.233	0.129	0.104	0.302	0.334
666	0.8524	0.231	0.125	0.106	0.337	0.341
The mean value of the eight last results						0.307

At room temperature Renninger has obtained

$$M = 1.15\,\frac{\sin^2 v_0}{\lambda^2}\,A^{-2} \quad \text{corresponding to } \Theta = 319°\,\mathrm{K}.$$

Correction for the influence of the diffuse scattering gives

$$M = 1.30\,\frac{\sin^2 v_0}{\lambda^2}\,A^{-2} \quad \text{corresponding to } \Theta = 302°\,\mathrm{K}.$$

From measurements of the specific heats we have $\Theta = 281°\,\mathrm{K}$

and calculations from the elastic constants [9] give $\Theta = 303°\,\mathrm{K}$.

The value obtained from specific heats is, however, a mean value over a large temperature range, and the value $\Theta = 303°\,\mathrm{K}$ is based upon a Debye frequency distribution. Thus the perfect agreement between the latter and the value obtained from

Renninger's measurements after correction for the diffuse scattering might be accidental, but anyhow it is apparent that the high value of 319° K can be accounted for by considering the diffuse scattering.[1]

Discussion of the results

The approximation introduced by taking a mean value of the part of T_1 that depends on the direction of the vector g, means that we replace the real surfaces of equal diffusion by spheres. When we integrate over the whole parallelepiped around the reciprocal lattice point the errors must cancel each other more or less, but when the direction of g varies within a smaller solid angle, as is the case in calculating σ', a larger error may be introduced in the value of the integral. Renninger himself says that the area on his curves corresponding to $ABCD$ in Fig. 3 amounts to up to 15 % of the reflection curve, that is at the most 26 % of our calculated Bragg reflection. According to our calculations the correction σ' corresponds to up to 40 % of the real integrated Bragg reflection.

The measurements are made without taking account of the azimuth of the crystal. Thus, in Fig. 2 the reciprocal lattice may be turned around OM and the parallelepiped will occupy different regions in the reciprocal lattice. However, Renninger has observed that the occasional adjustment of the crystal influences the results of the measurements by about 5 %. These facts support the assumption that using the mean value $\mathcal{K}$ does not give any large error in the value of the integrated diffuse reflection, for if that value were very sensitive to the detailed shape of the surfaces of equal diffusion within the parallelepiped, the different adjustments of the crystal would give corresponding variations of the experimental results.

The above calculations from experimental results with allowance for diffuse scattering cannot pretend to give the M-values with any great accuracy, because the earlier measurements are not very good, and in correcting Renninger's measurements it is difficult to determine how much of the total diffuse scattering influences his results. It is evident, however, that the influence of the diffuse scattering is very large. Renninger's high value of the characteristic temperature of rock-salt must be due to that circumstance. The fact that the effect of the diffuse scattering can be written as a factor $\exp\left(\text{const}\,\frac{\sin^2 v_0}{\lambda^2}\right)$ explains the good agreement between Renninger's curves of the experimental F-factors and the curves of the theoretical values.

I am most indebted to the head of this institute, Professor Ivar Waller, for suggesting this investigation and for much valuable advice during the work.

Institute of Theoretical Physics, University of Uppsala, Sweden.

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[1] In a recent article [10] (which appeared when this paper was going to press) Blackman points out that Renninger's high value of the characteristic temperature of rock-salt cannot be explained from the theory of Bragg scattering.

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